



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2025 – 06:26 pm GMT

PDB ID : 9RK3 / pdb_00009rk3
Title : Soluble domain of kustd1480, a Rieske iron-sulfur cluster protein from *Kuene-
nia stuttgartiensis*
Authors : Hauser, D.; Barends, T.
Deposited on : 2025-06-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

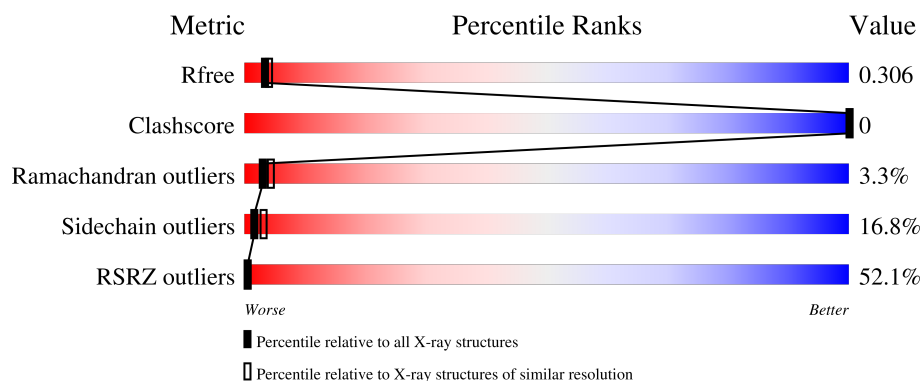
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1-A	117	<div> <div>50%</div> <div>80%</div> <div>20%</div> </div>
1	1-D	117	<div> <div>55%</div> <div>86%</div> <div>14%</div> </div>
1	2-A	117	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	2-D	117	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	3-A	117	<div> <div>79%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
1	3-D	117	 86% 12% .
1	4-A	117	 78% 21% .
1	4-D	117	 80% 19% .
1	5-A	117	 80% 19% .
1	5-D	117	 85% 15% .
1	6-A	117	 82% 18%
1	6-D	117	 86% 13% .
1	7-A	117	 80% 18% ..
1	7-D	117	 85% 15%
1	8-A	117	 80% 19% .
1	8-D	117	 85% 13% ..

2 Entry composition [i](#)

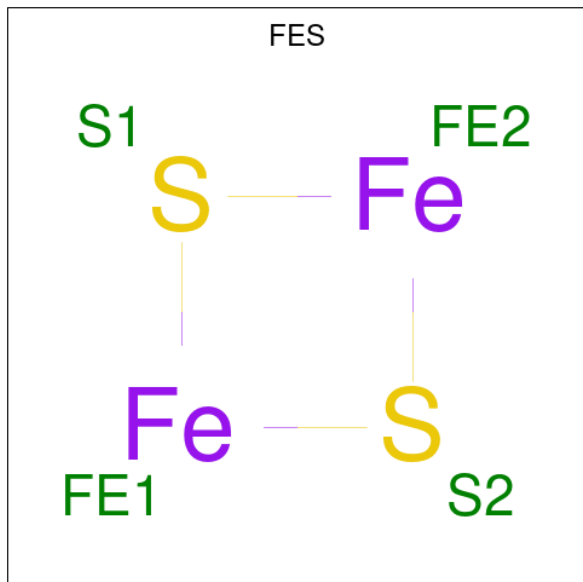
There are 3 unique types of molecules in this entry. The entry contains 29497 atoms, of which 14400 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	2-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	3-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	4-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	5-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	6-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	7-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	8-A	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	1-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	2-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	3-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	4-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	5-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	6-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	7-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			
1	8-D	117	Total	C	H	N	O	S	0	0	0
			1828	593	900	160	171	4			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	Fe	S	0	0
			4	2	2		
2	2-A	1	Total	Fe	S	0	0
			4	2	2		
2	3-A	1	Total	Fe	S	0	0
			4	2	2		
2	4-A	1	Total	Fe	S	0	0
			4	2	2		
2	5-A	1	Total	Fe	S	0	0
			4	2	2		
2	6-A	1	Total	Fe	S	0	0
			4	2	2		
2	7-A	1	Total	Fe	S	0	0
			4	2	2		
2	8-A	1	Total	Fe	S	0	0
			4	2	2		
2	1-D	1	Total	Fe	S	0	0
			4	2	2		
2	2-D	1	Total	Fe	S	0	0
			4	2	2		
2	3-D	1	Total	Fe	S	0	0
			4	2	2		
2	4-D	1	Total	Fe	S	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	5-D	1	Total 4	Fe 2	S 2	0	0
2	6-D	1	Total 4	Fe 2	S 2	0	0
2	7-D	1	Total 4	Fe 2	S 2	0	0
2	8-D	1	Total 4	Fe 2	S 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	17	Total 17	O 17	0	0
3	2-A	13	Total 13	O 13	0	0
3	3-A	13	Total 13	O 13	0	0
3	4-A	16	Total 16	O 16	0	0
3	5-A	15	Total 15	O 15	0	0
3	6-A	18	Total 18	O 18	0	0
3	7-A	15	Total 15	O 15	0	0
3	8-A	16	Total 16	O 16	0	0
3	1-D	8	Total 8	O 8	0	0
3	2-D	7	Total 7	O 7	0	0
3	3-D	6	Total 6	O 6	0	0
3	4-D	8	Total 8	O 8	0	0
3	5-D	8	Total 8	O 8	0	0
3	6-D	9	Total 9	O 9	0	0
3	7-D	8	Total 8	O 8	0	0

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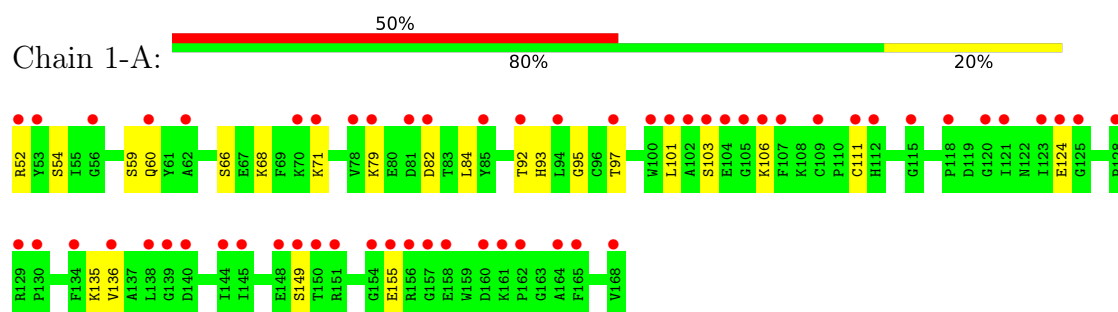
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	8-D	8	Total	O	0	0
			8	8		

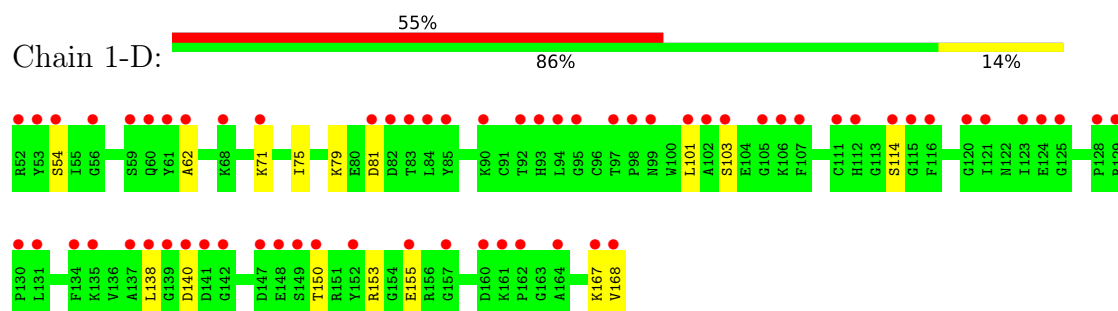
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

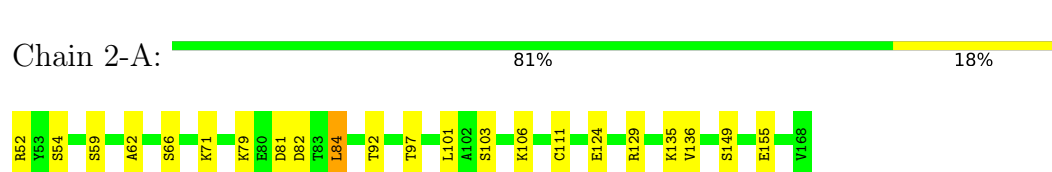
- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)



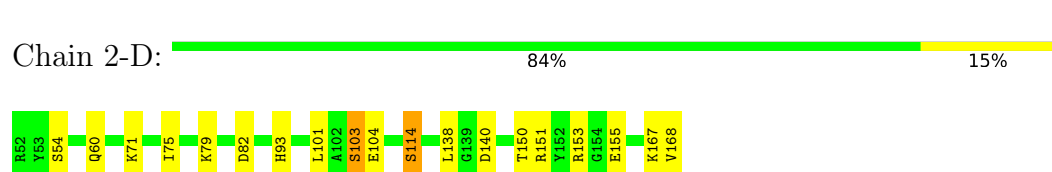
- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)




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Chain 3-A:  79% 21%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 3-D:  86% 12%




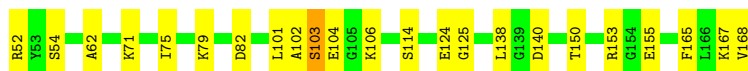
- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 4-A:  78% 21%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 4-D:  80% 19%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 5-A:  80% 19%




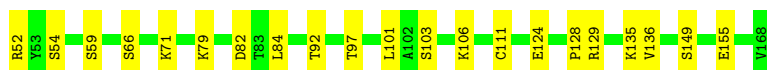
- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 5-D:  85% 15%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 6-A:  82% 18%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 6-D:  86% 13% .




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 7-A:  80% 18% ..




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 7-D:  85% 15%




- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 8-A:  80% 19% .



- Molecule 1: Similar to Rieske 2Fe-2S iron sulfur protein (Cytochrome b6-F complex)

Chain 8-D:  85% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.20Å 76.15Å 79.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.50 39.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.7 (39.51-2.50) 93.8 (39.51-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.221 , 0.276 0.253 , 0.306	Depositor DCC
R_{free} test set	1298 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.937	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.05 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29497	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9720e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.30	0/954	0.30	0/1286
1	1-D	0.28	0/954	0.28	0/1286
1	2-A	0.30	0/954	0.30	0/1286
1	2-D	0.28	0/954	0.28	0/1286
1	3-A	0.30	0/954	0.30	0/1286
1	3-D	0.28	0/954	0.28	0/1286
1	4-A	0.30	0/954	0.30	0/1286
1	4-D	0.28	0/954	0.28	0/1286
1	5-A	0.30	0/954	0.30	0/1286
1	5-D	0.28	0/954	0.28	0/1286
1	6-A	0.30	0/954	0.30	0/1286
1	6-D	0.28	0/954	0.28	0/1286
1	7-A	0.30	0/954	0.30	0/1286
1	7-D	0.28	0/954	0.28	0/1286
1	8-A	0.30	0/954	0.30	0/1286
1	8-D	0.28	0/954	0.28	0/1286
All	All	0.29	0/15264	0.29	0/20576

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-A	0	1
1	2-D	0	2
1	3-A	0	1
1	3-D	0	1
1	4-A	0	2
1	4-D	0	3
1	5-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	5-D	0	1
1	6-A	0	1
1	6-D	0	1
1	7-A	0	3
1	7-D	0	1
1	8-A	0	2
1	8-D	0	3
All	All	0	23

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2-A	129	ARG	Sidechain
1	2-D	114	SER	Peptide
1	2-D	82	ASP	Peptide
1	3-A	151	ARG	Sidechain
1	3-D	160	ASP	Peptide
1	4-A	141	ASP	Peptide
1	4-A	156	ARG	Sidechain
1	4-D	106	LYS	Peptide
1	4-D	124	GLU	Peptide
1	4-D	52	ARG	Sidechain
1	5-A	150	THR	Peptide
1	5-D	82	ASP	Peptide
1	6-A	129	ARG	Sidechain
1	6-D	140	ASP	Peptide
1	7-A	160	ASP	Peptide
1	7-A	52	ARG	Sidechain
1	7-A	82	ASP	Peptide
1	7-D	52	ARG	Sidechain
1	8-A	156	ARG	Sidechain
1	8-A	52	ARG	Sidechain
1	8-D	129	ARG	Sidechain
1	8-D	70	LYS	Peptide
1	8-D	71	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	928	900	900	0	0
1	1-D	928	900	900	0	0
1	2-A	928	900	900	0	0
1	2-D	928	900	900	0	0
1	3-A	928	900	900	0	0
1	3-D	928	900	900	0	0
1	4-A	928	900	900	0	0
1	4-D	928	900	900	0	0
1	5-A	928	900	900	0	0
1	5-D	928	900	900	0	0
1	6-A	928	900	900	0	0
1	6-D	928	900	900	0	0
1	7-A	928	900	900	0	0
1	7-D	928	900	900	0	0
1	8-A	928	900	900	0	0
1	8-D	928	900	900	0	0
2	1-A	4	0	0	0	0
2	1-D	4	0	0	0	0
2	2-A	4	0	0	0	0
2	2-D	4	0	0	0	0
2	3-A	4	0	0	0	0
2	3-D	4	0	0	0	0
2	4-A	4	0	0	0	0
2	4-D	4	0	0	0	0
2	5-A	4	0	0	0	0
2	5-D	4	0	0	0	0
2	6-A	4	0	0	0	0
2	6-D	4	0	0	0	0
2	7-A	4	0	0	0	0
2	7-D	4	0	0	0	0
2	8-A	4	0	0	0	0
2	8-D	4	0	0	0	0
3	1-A	17	0	0	0	0
3	1-D	8	0	0	0	0
3	2-A	13	0	0	0	0
3	2-D	7	0	0	0	0
3	3-A	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3-D	6	0	0	0	0
3	4-A	16	0	0	0	0
3	4-D	8	0	0	0	0
3	5-A	15	0	0	0	0
3	5-D	8	0	0	0	0
3	6-A	18	0	0	0	0
3	6-D	9	0	0	0	0
3	7-A	15	0	0	0	0
3	7-D	8	0	0	0	0
3	8-A	16	0	0	0	0
3	8-D	8	0	0	0	0
All	All	15097	14400	14400	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	115/117 (98%)	102 (89%)	9 (8%)	4 (4%)	3	4
1	1-D	115/117 (98%)	98 (85%)	15 (13%)	2 (2%)	7	14
1	2-A	115/117 (98%)	98 (85%)	14 (12%)	3 (3%)	4	7
1	2-D	115/117 (98%)	98 (85%)	12 (10%)	5 (4%)	2	3
1	3-A	115/117 (98%)	96 (84%)	14 (12%)	5 (4%)	2	3
1	3-D	115/117 (98%)	105 (91%)	7 (6%)	3 (3%)	4	7
1	4-A	115/117 (98%)	94 (82%)	14 (12%)	7 (6%)	1	1
1	4-D	115/117 (98%)	97 (84%)	11 (10%)	7 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-A	115/117 (98%)	94 (82%)	17 (15%)	4 (4%)	3	4
1	5-D	115/117 (98%)	102 (89%)	9 (8%)	4 (4%)	3	4
1	6-A	115/117 (98%)	96 (84%)	18 (16%)	1 (1%)	14	28
1	6-D	115/117 (98%)	103 (90%)	10 (9%)	2 (2%)	7	14
1	7-A	115/117 (98%)	100 (87%)	11 (10%)	4 (4%)	3	4
1	7-D	115/117 (98%)	100 (87%)	12 (10%)	3 (3%)	4	7
1	8-A	115/117 (98%)	98 (85%)	14 (12%)	3 (3%)	4	7
1	8-D	115/117 (98%)	106 (92%)	6 (5%)	3 (3%)	4	7
All	All	1840/1872 (98%)	1587 (86%)	193 (10%)	60 (3%)	3	4

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	68	LYS
1	1-D	62	ALA
1	2-D	104	GLU
1	2-D	151	ARG
1	3-A	93	HIS
1	3-A	104	GLU
1	3-A	114	SER
1	4-A	103	SER
1	4-A	104	GLU
1	4-A	155	GLU
1	4-D	103	SER
1	4-D	104	GLU
1	4-D	125	GLY
1	5-A	104	GLU
1	6-D	141	ASP
1	7-A	82	ASP
1	7-D	104	GLU
1	8-D	71	LYS
1	1-A	60	GLN
1	2-A	81	ASP
1	2-D	60	GLN
1	2-D	93	HIS
1	2-D	103	SER
1	4-A	93	HIS
1	5-D	83	THR
1	7-A	157	GLY

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Mol	Chain	Res	Type
1	7-A	158	GLU
1	7-D	60	GLN
1	7-D	93	HIS
1	8-A	81	ASP
1	8-D	103	SER
1	1-D	81	ASP
1	3-A	159	TRP
1	3-D	114	SER
1	3-D	160	ASP
1	4-D	82	ASP
1	4-D	165	PHE
1	5-D	82	ASP
1	2-A	84	LEU
1	4-A	60	GLN
1	4-D	62	ALA
1	5-A	60	GLN
1	5-A	103	SER
1	5-D	60	GLN
1	5-D	81	ASP
1	8-A	60	GLN
1	8-A	93	HIS
1	8-D	93	HIS
1	1-A	93	HIS
1	2-A	62	ALA
1	3-A	157	GLY
1	4-D	102	ALA
1	7-A	93	HIS
1	1-A	95	GLY
1	3-D	93	HIS
1	4-A	158	GLU
1	5-A	126	PRO
1	4-A	128	PRO
1	6-A	128	PRO
1	6-D	139	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	1-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	2-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	2-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	3-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	3-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	4-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	4-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	5-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	5-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	6-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	6-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	7-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	7-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
1	8-A	98/98 (100%)	79 (81%)	19 (19%)	1	2
1	8-D	98/98 (100%)	84 (86%)	14 (14%)	2	5
All	All	1568/1568 (100%)	1304 (83%)	264 (17%)	1	3

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	52	ARG
1	1-A	54	SER
1	1-A	59	SER
1	1-A	66	SER
1	1-A	71	LYS
1	1-A	79	LYS
1	1-A	82	ASP
1	1-A	84	LEU
1	1-A	92	THR
1	1-A	97	THR
1	1-A	101	LEU
1	1-A	103	SER
1	1-A	106	LYS
1	1-A	111	CYS
1	1-A	124	GLU
1	1-A	135	LYS

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Mol	Chain	Res	Type
1	1-A	136	VAL
1	1-A	149	SER
1	1-A	155	GLU
1	1-D	54	SER
1	1-D	71	LYS
1	1-D	75	ILE
1	1-D	79	LYS
1	1-D	101	LEU
1	1-D	103	SER
1	1-D	114	SER
1	1-D	138	LEU
1	1-D	140	ASP
1	1-D	150	THR
1	1-D	153	ARG
1	1-D	155	GLU
1	1-D	167	LYS
1	1-D	168	VAL
1	2-A	52	ARG
1	2-A	54	SER
1	2-A	59	SER
1	2-A	66	SER
1	2-A	71	LYS
1	2-A	79	LYS
1	2-A	82	ASP
1	2-A	84	LEU
1	2-A	92	THR
1	2-A	97	THR
1	2-A	101	LEU
1	2-A	103	SER
1	2-A	106	LYS
1	2-A	111	CYS
1	2-A	124	GLU
1	2-A	135	LYS
1	2-A	136	VAL
1	2-A	149	SER
1	2-A	155	GLU
1	2-D	54	SER
1	2-D	71	LYS
1	2-D	75	ILE
1	2-D	79	LYS
1	2-D	101	LEU
1	2-D	103	SER

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Mol	Chain	Res	Type
1	2-D	114	SER
1	2-D	138	LEU
1	2-D	140	ASP
1	2-D	150	THR
1	2-D	153	ARG
1	2-D	155	GLU
1	2-D	167	LYS
1	2-D	168	VAL
1	3-A	52	ARG
1	3-A	54	SER
1	3-A	59	SER
1	3-A	66	SER
1	3-A	71	LYS
1	3-A	79	LYS
1	3-A	82	ASP
1	3-A	84	LEU
1	3-A	92	THR
1	3-A	97	THR
1	3-A	101	LEU
1	3-A	103	SER
1	3-A	106	LYS
1	3-A	111	CYS
1	3-A	124	GLU
1	3-A	135	LYS
1	3-A	136	VAL
1	3-A	149	SER
1	3-A	155	GLU
1	3-D	54	SER
1	3-D	71	LYS
1	3-D	75	ILE
1	3-D	79	LYS
1	3-D	101	LEU
1	3-D	103	SER
1	3-D	114	SER
1	3-D	138	LEU
1	3-D	140	ASP
1	3-D	150	THR
1	3-D	153	ARG
1	3-D	155	GLU
1	3-D	167	LYS
1	3-D	168	VAL
1	4-A	52	ARG

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Mol	Chain	Res	Type
1	4-A	54	SER
1	4-A	59	SER
1	4-A	66	SER
1	4-A	71	LYS
1	4-A	79	LYS
1	4-A	82	ASP
1	4-A	84	LEU
1	4-A	92	THR
1	4-A	97	THR
1	4-A	101	LEU
1	4-A	103	SER
1	4-A	106	LYS
1	4-A	111	CYS
1	4-A	124	GLU
1	4-A	135	LYS
1	4-A	136	VAL
1	4-A	149	SER
1	4-A	155	GLU
1	4-D	54	SER
1	4-D	71	LYS
1	4-D	75	ILE
1	4-D	79	LYS
1	4-D	101	LEU
1	4-D	103	SER
1	4-D	114	SER
1	4-D	138	LEU
1	4-D	140	ASP
1	4-D	150	THR
1	4-D	153	ARG
1	4-D	155	GLU
1	4-D	167	LYS
1	4-D	168	VAL
1	5-A	52	ARG
1	5-A	54	SER
1	5-A	59	SER
1	5-A	66	SER
1	5-A	71	LYS
1	5-A	79	LYS
1	5-A	82	ASP
1	5-A	84	LEU
1	5-A	92	THR
1	5-A	97	THR

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Mol	Chain	Res	Type
1	5-A	101	LEU
1	5-A	103	SER
1	5-A	106	LYS
1	5-A	111	CYS
1	5-A	124	GLU
1	5-A	135	LYS
1	5-A	136	VAL
1	5-A	149	SER
1	5-A	155	GLU
1	5-D	54	SER
1	5-D	71	LYS
1	5-D	75	ILE
1	5-D	79	LYS
1	5-D	101	LEU
1	5-D	103	SER
1	5-D	114	SER
1	5-D	138	LEU
1	5-D	140	ASP
1	5-D	150	THR
1	5-D	153	ARG
1	5-D	155	GLU
1	5-D	167	LYS
1	5-D	168	VAL
1	6-A	52	ARG
1	6-A	54	SER
1	6-A	59	SER
1	6-A	66	SER
1	6-A	71	LYS
1	6-A	79	LYS
1	6-A	82	ASP
1	6-A	84	LEU
1	6-A	92	THR
1	6-A	97	THR
1	6-A	101	LEU
1	6-A	103	SER
1	6-A	106	LYS
1	6-A	111	CYS
1	6-A	124	GLU
1	6-A	135	LYS
1	6-A	136	VAL
1	6-A	149	SER
1	6-A	155	GLU

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Mol	Chain	Res	Type
1	6-D	54	SER
1	6-D	71	LYS
1	6-D	75	ILE
1	6-D	79	LYS
1	6-D	101	LEU
1	6-D	103	SER
1	6-D	114	SER
1	6-D	138	LEU
1	6-D	140	ASP
1	6-D	150	THR
1	6-D	153	ARG
1	6-D	155	GLU
1	6-D	167	LYS
1	6-D	168	VAL
1	7-A	52	ARG
1	7-A	54	SER
1	7-A	59	SER
1	7-A	66	SER
1	7-A	71	LYS
1	7-A	79	LYS
1	7-A	82	ASP
1	7-A	84	LEU
1	7-A	92	THR
1	7-A	97	THR
1	7-A	101	LEU
1	7-A	103	SER
1	7-A	106	LYS
1	7-A	111	CYS
1	7-A	124	GLU
1	7-A	135	LYS
1	7-A	136	VAL
1	7-A	149	SER
1	7-A	155	GLU
1	7-D	54	SER
1	7-D	71	LYS
1	7-D	75	ILE
1	7-D	79	LYS
1	7-D	101	LEU
1	7-D	103	SER
1	7-D	114	SER
1	7-D	138	LEU
1	7-D	140	ASP

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Mol	Chain	Res	Type
1	7-D	150	THR
1	7-D	153	ARG
1	7-D	155	GLU
1	7-D	167	LYS
1	7-D	168	VAL
1	8-A	52	ARG
1	8-A	54	SER
1	8-A	59	SER
1	8-A	66	SER
1	8-A	71	LYS
1	8-A	79	LYS
1	8-A	82	ASP
1	8-A	84	LEU
1	8-A	92	THR
1	8-A	97	THR
1	8-A	101	LEU
1	8-A	103	SER
1	8-A	106	LYS
1	8-A	111	CYS
1	8-A	124	GLU
1	8-A	135	LYS
1	8-A	136	VAL
1	8-A	149	SER
1	8-A	155	GLU
1	8-D	54	SER
1	8-D	71	LYS
1	8-D	75	ILE
1	8-D	79	LYS
1	8-D	101	LEU
1	8-D	103	SER
1	8-D	114	SER
1	8-D	138	LEU
1	8-D	140	ASP
1	8-D	150	THR
1	8-D	153	ARG
1	8-D	155	GLU
1	8-D	167	LYS
1	8-D	168	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	72	GLN
1	1-D	60	GLN
1	2-A	72	GLN
1	2-A	143	GLN
1	3-A	60	GLN
1	3-A	72	GLN
1	3-A	99	ASN
1	4-A	60	GLN
1	4-A	72	GLN
1	4-D	143	GLN
1	5-A	72	GLN
1	5-D	99	ASN
1	7-A	60	GLN
1	7-A	112	HIS
1	7-D	60	GLN
1	8-A	72	GLN
1	8-D	60	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FES	5-D	201	1	0,4,4	-	-	-		
2	FES	2-D	201	1	0,4,4	-	-	-		
2	FES	7-D	201	1	0,4,4	-	-	-		
2	FES	6-A	201	1	0,4,4	-	-	-		
2	FES	3-A	201	1	0,4,4	-	-	-		
2	FES	1-A	201	1	0,4,4	-	-	-		
2	FES	4-A	201	1	0,4,4	-	-	-		
2	FES	3-D	201	1	0,4,4	-	-	-		
2	FES	4-D	201	1	0,4,4	-	-	-		
2	FES	6-D	201	1	0,4,4	-	-	-		
2	FES	1-D	201	1	0,4,4	-	-	-		
2	FES	8-D	201	1	0,4,4	-	-	-		
2	FES	7-A	201	1	0,4,4	-	-	-		
2	FES	8-A	201	1	0,4,4	-	-	-		
2	FES	2-A	201	1	0,4,4	-	-	-		
2	FES	5-A	201	1	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FES	5-D	201	1	-	-	0/1/1/1
2	FES	2-D	201	1	-	-	0/1/1/1
2	FES	7-D	201	1	-	-	0/1/1/1
2	FES	6-A	201	1	-	-	0/1/1/1
2	FES	3-A	201	1	-	-	0/1/1/1
2	FES	1-A	201	1	-	-	0/1/1/1
2	FES	4-A	201	1	-	-	0/1/1/1
2	FES	3-D	201	1	-	-	0/1/1/1
2	FES	4-D	201	1	-	-	0/1/1/1
2	FES	6-D	201	1	-	-	0/1/1/1
2	FES	1-D	201	1	-	-	0/1/1/1
2	FES	8-D	201	1	-	-	0/1/1/1
2	FES	7-A	201	1	-	-	0/1/1/1
2	FES	8-A	201	1	-	-	0/1/1/1
2	FES	2-A	201	1	-	-	0/1/1/1
2	FES	5-A	201	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

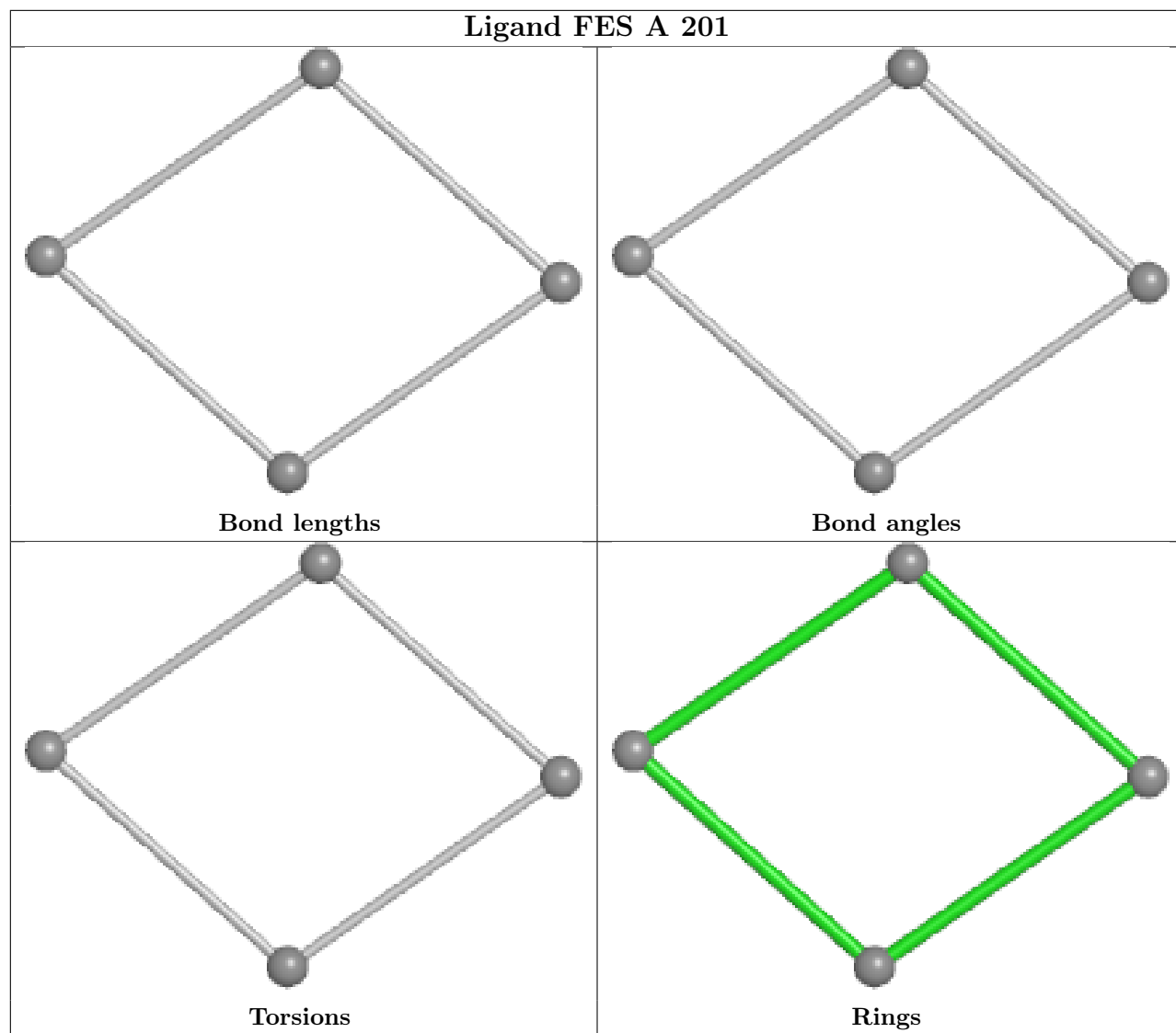
There are no chirality outliers.

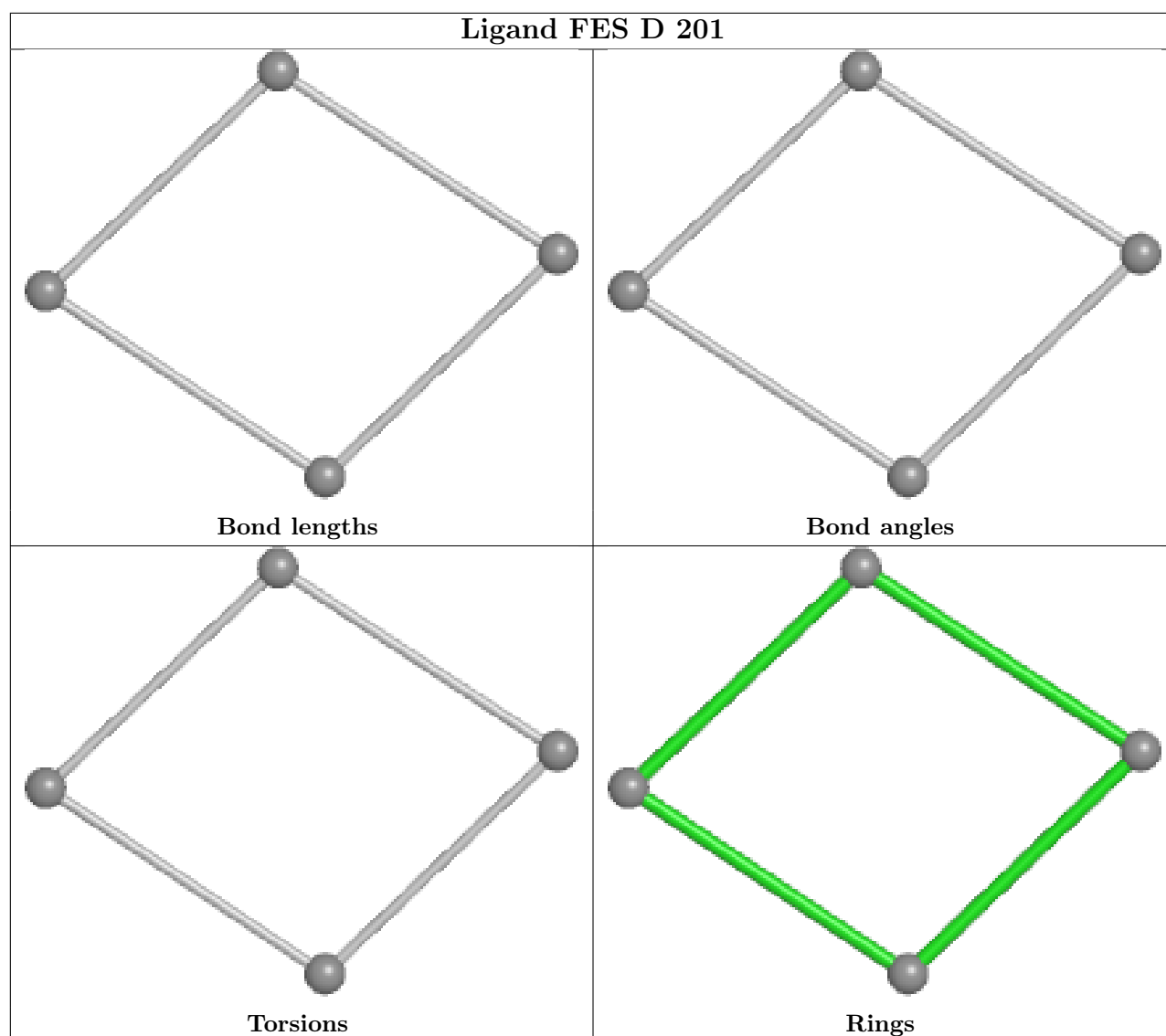
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.







5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	117/117 (100%)	2.24	58 (49%)  	4, 6, 8, 8	117 (100%)
1	1-D	117/117 (100%)	2.17	64 (54%)  	4, 5, 7, 8	117 (100%)
1	2-A	0/117	-	-	-	-
1	2-D	0/117	-	-	-	-
1	3-A	0/117	-	-	-	-
1	3-D	0/117	-	-	-	-
1	4-A	0/117	-	-	-	-
1	4-D	0/117	-	-	-	-
1	5-A	0/117	-	-	-	-
1	5-D	0/117	-	-	-	-
1	6-A	0/117	-	-	-	-
1	6-D	0/117	-	-	-	-
1	7-A	0/117	-	-	-	-
1	7-D	0/117	-	-	-	-
1	8-A	0/117	-	-	-	-
1	8-D	0/117	-	-	-	-
All	All	234/1872 (12%)	2.20	122 (52%)  	4, 6, 8, 8	234 (100%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	150	THR	7.0
1	1-A	149	SER	7.0
1	1-A	94	LEU	6.6
1	1-A	157	GLY	6.0
1	1-A	160	ASP	5.6
1	1-D	155	GLU	5.5
1	1-D	97	THR	5.3
1	1-A	156	ARG	5.1
1	1-A	111	CYS	4.7
1	1-D	125	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	1-D	92	THR	4.3
1	1-A	155	GLU	4.3
1	1-A	82	ASP	4.3
1	1-A	120	GLY	4.1
1	1-D	82	ASP	4.1
1	1-D	71	LYS	3.9
1	1-D	101	LEU	3.9
1	1-D	120	GLY	3.9
1	1-D	54	SER	3.8
1	1-D	124	GLU	3.7
1	1-A	168	VAL	3.7
1	1-D	138	LEU	3.7
1	1-A	92	THR	3.7
1	1-D	52	ARG	3.5
1	1-A	161	LYS	3.5
1	1-A	101	LEU	3.5
1	1-D	162	PRO	3.4
1	1-D	168	VAL	3.4
1	1-A	134	PHE	3.4
1	1-D	141	ASP	3.3
1	1-D	60	GLN	3.3
1	1-A	125	GLY	3.3
1	1-A	71	LYS	3.3
1	1-D	150	THR	3.3
1	1-A	79	LYS	3.2
1	1-A	128	PRO	3.2
1	1-D	131	LEU	3.2
1	1-D	53	TYR	3.2
1	1-D	147	ASP	3.1
1	1-D	111	CYS	3.1
1	1-A	53	TYR	3.1
1	1-D	160	ASP	3.1
1	1-A	107	PHE	3.1
1	1-D	90	LYS	3.1
1	1-A	100	TRP	3.1
1	1-A	136	VAL	3.0
1	1-D	112	HIS	3.0
1	1-D	128	PRO	3.0
1	1-D	83	THR	3.0
1	1-A	52	ARG	3.0
1	1-D	93	HIS	3.0
1	1-A	105	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	154	GLY	2.9
1	1-A	102	ALA	2.9
1	1-D	59	SER	2.9
1	1-D	152	TYR	2.9
1	1-A	103	SER	2.8
1	1-D	56	GLY	2.8
1	1-D	81	ASP	2.7
1	1-A	129	ARG	2.7
1	1-D	129	ARG	2.7
1	1-A	97	THR	2.7
1	1-A	106	LYS	2.7
1	1-D	106	LYS	2.7
1	1-A	140	ASP	2.7
1	1-D	99	ASN	2.7
1	1-A	56	GLY	2.7
1	1-D	105	GLY	2.7
1	1-D	134	PHE	2.6
1	1-D	140	ASP	2.6
1	1-A	124	GLU	2.5
1	1-A	85	TYR	2.5
1	1-D	167	LYS	2.5
1	1-D	114	SER	2.5
1	1-A	62	ALA	2.5
1	1-A	118	PRO	2.5
1	1-D	121	ILE	2.5
1	1-D	161	LYS	2.5
1	1-D	62	ALA	2.5
1	1-D	95	GLY	2.5
1	1-D	139	GLY	2.5
1	1-D	102	ALA	2.4
1	1-D	148	GLU	2.4
1	1-A	138	LEU	2.4
1	1-D	61	TYR	2.4
1	1-D	157	GLY	2.4
1	1-A	60	GLN	2.4
1	1-A	162	PRO	2.4
1	1-D	103	SER	2.4
1	1-D	116	PHE	2.3
1	1-D	149	SER	2.3
1	1-A	104	GLU	2.3
1	1-D	84	LEU	2.3
1	1-D	135	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	165	PHE	2.2
1	1-A	81	ASP	2.2
1	1-A	148	GLU	2.2
1	1-D	107	PHE	2.2
1	1-D	85	TYR	2.2
1	1-D	115	GLY	2.2
1	1-A	109	CYS	2.2
1	1-A	112	HIS	2.2
1	1-A	164	ALA	2.2
1	1-A	158	GLU	2.2
1	1-A	78	VAL	2.2
1	1-D	98	PRO	2.1
1	1-D	130	PRO	2.1
1	1-A	144	ILE	2.1
1	1-A	145	ILE	2.1
1	1-A	139	GLY	2.1
1	1-A	130	PRO	2.1
1	1-A	121	ILE	2.1
1	1-A	123	ILE	2.1
1	1-D	164	ALA	2.1
1	1-D	68	LYS	2.1
1	1-D	123	ILE	2.1
1	1-D	94	LEU	2.0
1	1-A	151	ARG	2.0
1	1-D	137	ALA	2.0
1	1-A	70	LYS	2.0
1	1-A	115	GLY	2.0
1	1-D	142	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

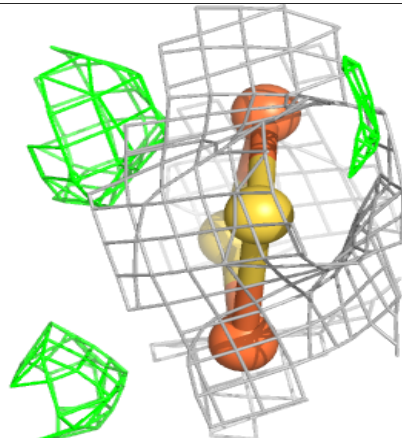
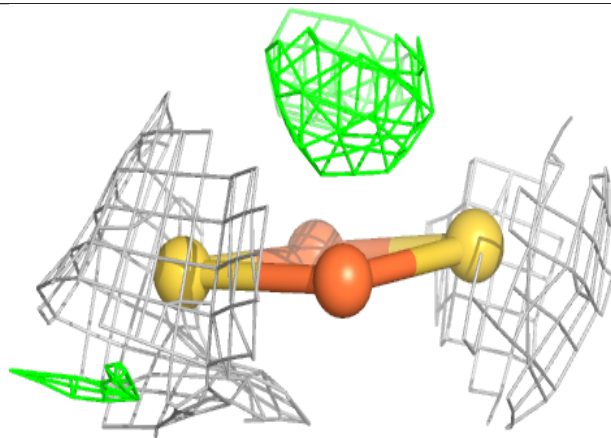
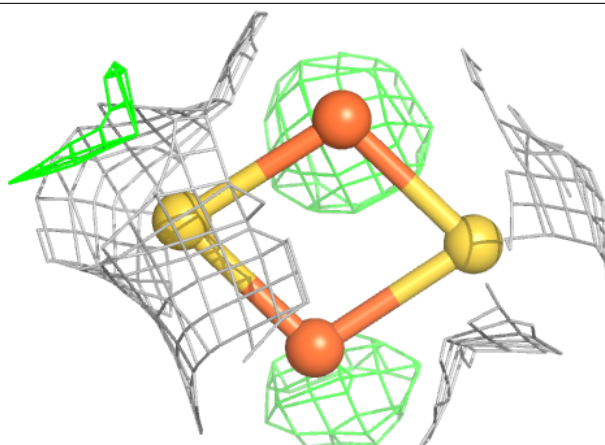
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FES	1-A	201	4/4	0.92	0.09	45,47,49,51	4
2	FES	2-A	201	4/4	-	-	45,47,49,51	4
2	FES	3-A	201	4/4	-	-	45,47,49,51	4
2	FES	4-A	201	4/4	-	-	45,47,49,51	4
2	FES	5-A	201	4/4	-	-	45,47,49,51	4
2	FES	6-A	201	4/4	-	-	45,47,49,51	4
2	FES	7-A	201	4/4	-	-	45,47,49,51	4
2	FES	8-A	201	4/4	-	-	45,47,49,51	4
2	FES	1-D	201	4/4	0.92	0.08	44,45,48,49	4
2	FES	2-D	201	4/4	-	-	44,45,48,49	4
2	FES	3-D	201	4/4	-	-	44,45,48,49	4
2	FES	4-D	201	4/4	-	-	44,45,48,49	4
2	FES	5-D	201	4/4	-	-	44,45,48,49	4
2	FES	6-D	201	4/4	-	-	44,45,48,49	4
2	FES	7-D	201	4/4	-	-	44,45,48,49	4
2	FES	8-D	201	4/4	-	-	44,45,48,49	4

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

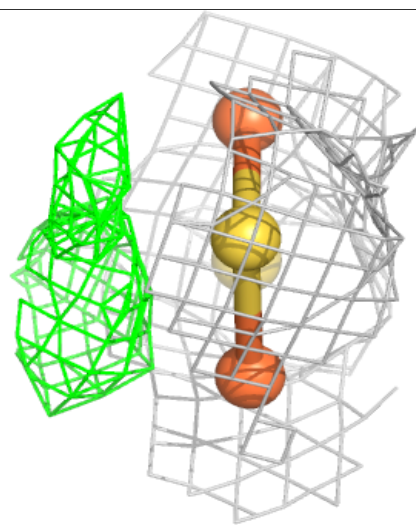
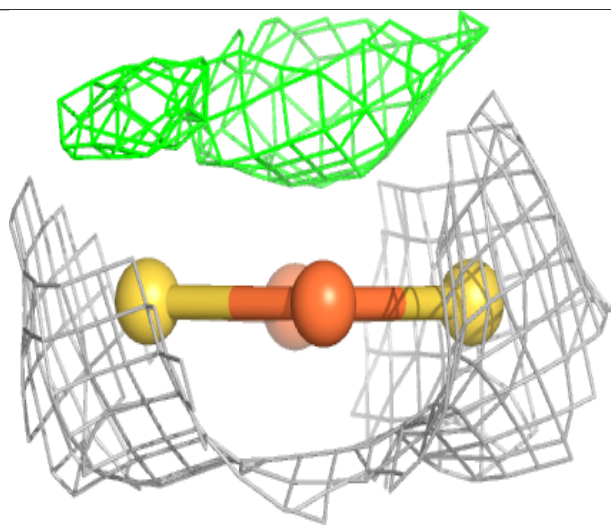
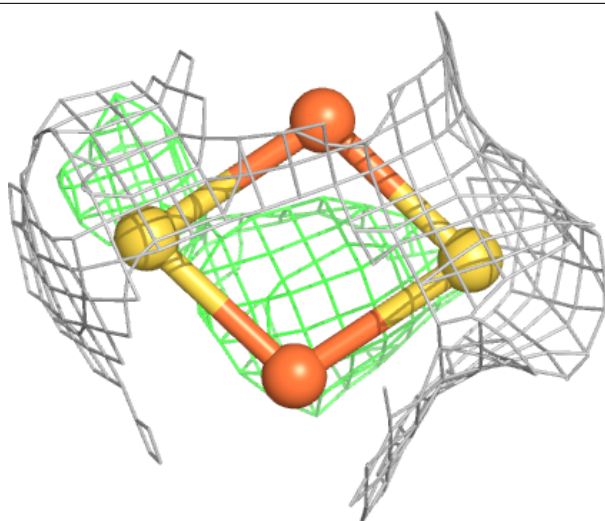
Electron density around FES A 201:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FES D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.